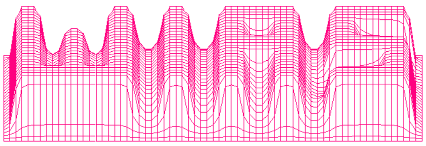
Electro–reaction–diffusion systems in heterostructures

Annegret Glitzky, Rolf Hünlich



Weierstrass Institute for Applied Analysis and Stochastics
Mohrenstrasse 39, D – 10117 Berlin
glitzky@wias–berlin.de

Electro-reaction-diffusion system

X_i	species, $i = 1, \dots, M$	q_i	charges
v_i	chem. pot.	$u_i = \overline{u}_i\, e^{v_i}$	concentrations
v_0	electrostat. pot.	$\zeta_i := v_i + q_i v_0$	electrochem. pot.

mass fluxes:

$$j_i = -D_i\, u_i \nabla \zeta_i = -D_i\, u_i \nabla (v_i + q_i v_0)$$

reactions:

$$\alpha_1 X_1 + \cdots + \alpha_M X_M \rightleftharpoons \beta_1 X_1 + \cdots + \beta_M X_M$$

reaction rates in Ω, at Γ:

$$R_i = \sum_{(\alpha,\,\beta)\in\mathcal{R}} k_{\alpha\beta} \Big(\prod_{k=1}^{M} e^{\zeta_k \alpha_k} - \prod_{k=1}^{M} e^{\zeta_k \beta_k} \Big)(\alpha_i - \beta_i)$$

differential equations:

$$\boxed{\begin{aligned}
\frac{\partial u_i}{\partial t} + \nabla \cdot j_i + R_i^\Omega &= 0 \quad \text{on } \mathbb{R}_+ \times \Omega \\
\nu \cdot j_i &= R_i^\Gamma \ \text{ on } \mathbb{R}_+ \times \Gamma \\
u_i(0) &= U_i \ \text{ on } \Omega, \quad i = 1, \dots, M, \\
-\nabla \cdot (\varepsilon \nabla v_0) &= f^\Omega + \sum_{i=1}^{M} q_i u_i \ \text{ on } \mathbb{R}_+ \times \Omega \\
\nu \cdot (\varepsilon \nabla v_0) + \tau v_0 &= f^\Gamma \ \text{ on } \mathbb{R}_+ \times \Gamma_N \\
v_0 &= v_D \ \text{ on } \mathbb{R}_+ \times \Gamma_D
\end{aligned}}$$

Weak formulation

variables:

$$v = (v_0, v_1, \ldots, v_M),\ \ u = (u_0, u_1, \ldots, u_M) \colon \mathbb{R}_+ \times \Omega \to \mathbb{R}^{M+1},$$

$$U = \Big(\sum_{i=1}^{M} q_i U_i, U_1, \ldots, U_M\Big)$$

operators:

$$A \colon X \cap L^\infty(\Omega, \mathbb{R}^{M+1}) \to X^*,\ \ E = (E_0, \ldots, E_M) \colon X \to X^*$$

$$X := H_0^1(\Omega \cup \Gamma_N) \times H^1(\Omega, \mathbb{R}^M)$$

Problem (P):

$$u'(t) + A\,v(t) = 0,\ \ u(t) = Ev(t) \text{ f.a.a. } t \in \mathbb{R}_+\,; \quad u(0) = U$$
$$u \in H^1_{\mathrm{loc}}(\mathbb{R}_+, X^*),\ \ v \in L^2_{\mathrm{loc}}(\mathbb{R}_+, X) \cap L^\infty_{\mathrm{loc}}(\mathbb{R}_+, L^\infty(\Omega, \mathbb{R}^{M+1}))$$

Theorem 1 (Steady states)

In some compatibility class defined by the initial value there is a unique steady state (u^*, v^*) to (P).

Energetic estimates

$\boldsymbol{E}$ strictly monotone potential operator with potential

$$\Phi : X \to \mathbb{R}$$

free energy $\quad F : X^* \to \overline{\mathbb{R}}, \quad F(u) := \Phi^*(u)$

$$F(u) = \int_\Omega \left\{ \frac{\varepsilon}{2} |\nabla v_0|^2 + \sum_{i=1}^{M} \left(u_i (\ln \frac{u_i}{\overline{u}_i} - 1) + \overline{u}_i \right) \right\} \mathrm{d}x + \int_{\Gamma_N} \frac{\tau}{2} v_0^2 \, \mathrm{d}\Gamma$$

where $E_0 v_0 = u_0$

Theorem 2 (Boundedness of the free energy)
If (u, v) is a solution to (P) then

$$F(u(t_2)) \le F(u(t_1)) \le F(U) \quad t_2 \ge t_1 \ge 0.$$

Theorem 3 (Exponential decay of the free energy)
There exist $c, \lambda > 0$ such that for any solution (u, v) to (P)

$$F(u(t)) - F(u^*) \le e^{-\lambda t} (F(U) - F(u^*)) \quad \forall t \ge 0.$$

Reference:
A. Glitzky and R. Hünlich, *Energetic estimates and asymptotics for electro–reaction–diffusion systems*, Z. Angew. Math. Mech. 77 (1997), 823–832.

Existence results

assume:

order of source terms of volume reactions ≤ 2,
order of source terms of boundary reac. $\leq 3/2$

Theorem 4 (Existence, uniqueness)
There exists a unique solution (u, v) to (P).

Theorem 5 (Global estimates, asymptotics)
Let (u, v) be the solution to (P). Then there exist constants c, $\lambda_p > 0$ depending only on the data such that

- $\sum_{i=0}^{M} \big(\|u_i(t)\|_{L^\infty} + \|v_i(t)\|_{L^\infty}\big) \leq c \qquad \forall t \in \mathbb{R}_+,$
- $\sum_{i=1}^{M} \|u_i(t) - u_i^*\|_{L^p} \leq c\, e^{-\lambda_p t} \quad \forall\, t \in \mathbb{R}_+,$
- $\sum_{i=0}^{M} \|v_i(t) - v_i^*\|_{L^p} \leq c\, e^{-\lambda_p t} \quad \forall t \in \mathbb{R}_+, \qquad$ where $p \in [1, +\infty)$.

References:

A. Glitzky and R. Hünlich, *Global estimates and asymptotics for electro–reaction–diffusion systems in heterostructures*, Applicable Analysis 66 (1997), 205–226.

A. Glitzky and R. Hünlich, *Electro–reaction–diffusion systems including cluster reactions of higher order*, Math. Nachr. (to appear).

Model reduction for partly fast kinetics

assumptions concerning

- subsets of fast volume reactions
- subsets of fast reactions on $\Omega_0 \subset \Omega$
- subsets of fast boundary reactions
- fast diffusion of some species
- combinations of the above cases

lead to states (u, v) where v lies in a linear subspace of X

$$v = L\widetilde{v}, \quad \widetilde{u} = L^* u, \quad (\widetilde{u}, \widetilde{v}) \in \widetilde{X} \times \widetilde{X}^*$$

$L\colon \widetilde{X} \to X$ has the properties:

- L linear, continuous, injective,
- Im L closed in X,
- $\Big\{v \in X\colon\ \zeta \in \Big[\mathrm{span}\big\{\alpha - \beta\colon (\alpha, \beta) \in \mathcal{R}\big\}\Big]^{\perp}\Big\} \subset \operatorname{Im} L$

by a projection scheme results Problem $(\widetilde{\mathrm{P}})$:

$$\widetilde{u}'(t) + L^* A L\, \widetilde{v}(t) = 0,\ \widetilde{u}(t) = L^* E L\, \widetilde{v}(t) \text{ f.a.a. } t \in \mathbb{R}_+,$$

$$\widetilde{u}(0) = L^* U,$$

$$\widetilde{u} \in H^1_{\mathrm{loc}}(\mathbb{R}_+, \widetilde{X}^*),\ \widetilde{v} \in L^2_{\mathrm{loc}}(\mathbb{R}_+, \widetilde{X}),$$

$$L\widetilde{v} \in L^2_{\mathrm{loc}}(\mathbb{R}_+, X) \cap L^\infty_{\mathrm{loc}}(\mathbb{R}_+, L^\infty(\Omega, \mathbb{R}^{M+1}))$$

Transfer of the convex structure from (P) to $(\widetilde{\mathrm{P}})$:

Theorem 6 (Steady states)
There exists a unique steady state $(\widetilde{u}^*, \widetilde{v}^*)$ to $(\widetilde{\mathrm{P}})$ and it holds $\widetilde{u}^* = L^* u^*$, $v^* = L\widetilde{v}^*$ where (u^*, v^*) is the steady state to (P).

$\widetilde{\Phi} \colon \widetilde{X} \to \mathbb{R}$

$$\boxed{\widetilde{\Phi}(\widetilde{v}) := \Phi(L\widetilde{v}), \quad \partial\widetilde{\Phi}(\widetilde{v}) = L^* E L\widetilde{v}}$$

free energy: $\widetilde{F} := \widetilde{\Phi}^*$,

if $\widetilde{F}$ is subdiff. in $\widetilde{u}$ $\Longrightarrow$

$$\widetilde{F}(\widetilde{u}) = F(u) \qquad \text{with } u = \partial\Phi(L\widetilde{v}) = Ev$$

Theorem 7 (Energetic estimates)
Along any solution $(\widetilde{u}, \widetilde{v})$ to $(\widetilde{\mathrm{P}})$ it holds

- $\widetilde{F}(\widetilde{u}(t_2)) \le \widetilde{F}(\widetilde{u}(t_1)) \le \widetilde{F}(L^* U) \quad 0 \le t_1 \le t_2,$

- $\widetilde{F}(\widetilde{u}(t)) - \widetilde{F}(\widetilde{u}^*) \le e^{-\lambda t}\big(\widetilde{F}(L^* U) - \widetilde{F}(\widetilde{u}^*)\big) \quad \forall t \in \mathbb{R}_+.$

Reference:
A. Glitzky and R. Hünlich, *Energetic estimates for electro–reaction–diffusion systems with partly fast kinetics*, in preparation.

Applications

- models with fast kinetic for electrons and holes:
  continuity equations for electrons and holes disappear,
  nonlinear Poisson equation and nonlocal condition
- reduction of pair diffusion models (Lang, Merz)
- further step by step reduction of model equations (e.g. fast pairing reactions in the pair diffusion model)

Open questions, problems

- existence results, global estimates for the reduced problem $(\widetilde{\mathrm{P}})$ can not be obtained by such a general scheme from results for the basic problem
- concrete structure of the reduced model equations can be complicated:
  strong coupling under the time derivative
  strongly coupled diffusion parts
  additional nonlinearities
  nonlocal expressions in volume or boundary terms
- models without diffusion for some species
- general reactions of higher order ?
- 3D ??

Comparison of the models

$(\widetilde{u}, \widetilde{v})$ solution to $(\widetilde{\mathrm{P}})$, (u, v) solution to (P)

reconstructed quantities:

$$\boxed{\breve{v} := L\widetilde{v}, \quad \breve{u} := EL\widetilde{v}}$$

steady states:

$$\boxed{\breve{v}^* := L\widetilde{v}^* = v^*, \quad \breve{u}^* := EL\widetilde{v}^* = u^*}$$

on trajectories of $(\widetilde{\mathrm{P}})$

$$\widetilde{F}(\widetilde{u}(t)) = F(\breve{u}(t)) \quad \text{f.a.a. } t \in \mathbb{R}_+$$

conclusions from energetic estimates for (P) and $(\widetilde{\mathrm{P}})$:

$$\boxed{\begin{aligned} &|F(\breve{u}(t)) - F(u(t))| \le ce^{-\lambda t}, \\ &\|\breve{v}_0(t) - v_0(t)\|_{H^1} \le ce^{-\lambda t/2}, \\ &\|\breve{u}_i(t) - u_i(t)\|_{L^1} \le ce^{-\lambda t/2} \qquad \text{f.a.a. } t \in \mathbb{R}_+ \end{aligned}}$$

Reference:

A. Glitzky and R. Hünlich, *Energetic estimates for electro–reaction–diffusion systems with partly fast kinetics*, in preparation.

Assumptions

Ω bounded Lipschitzian domain in $\mathbb{R}^2$, $\Gamma := \partial\Omega$,
Γ_D, Γ_N disjoint open subsets of Γ, $\Gamma = \overline{\Gamma_D} \cup \overline{\Gamma_N}$,
$\overline{\Gamma_D} \cap \overline{\Gamma_N}$ consists of finitely many points;

$q_i \in \mathbb{Z}$, $\overline{u}_i$, $U_i \in L^\infty(\Omega)$, $\overline{u}_i$, $U_i \geq c > 0$,
$D_i \in L^\infty(\Omega)$, $D_i \geq c > 0$, $i = 1, \ldots, M$;
$U_0 := \Sigma_{i=1}^{M} q_i U_i$, $q := (q_1, \ldots, q_M)$;
$\varepsilon \in L^\infty(\Omega)$, $\varepsilon \geq c > 0$, $\tau \in L^\infty_+(\Gamma_N)$, $\operatorname{mes}\Gamma_D + \|\tau\|_{L^1(\Gamma_N)} > 0$;

$\mathcal{R}^\Omega$, $\mathcal{R}^\Gamma$ finite subsets of $\mathbb{Z}^M_+ \times \mathbb{Z}^M_+$;
$(\alpha - \beta) \cdot q = 0 \;\; \forall (\alpha, \beta) \in \mathcal{R}^\Omega \cup \mathcal{R}^\Gamma$;
for $\Sigma = \Omega, \Gamma$ and $(\alpha, \beta) \in \mathcal{R}^\Sigma$ we define
$R^\Sigma_{\alpha\beta} := k^\Sigma_{\alpha\beta}(x, y)\,(e^{\alpha\cdot\zeta} - e^{\beta\cdot\zeta})$,
$x \in \Sigma$, $y = (y_0, y_1, \cdots, y_M) \in \mathbb{R}^{M+1}$,
$\zeta_i := y_i + q_i y_0$, $i = 1, \ldots, M$, where
$k^\Sigma_{\alpha\beta} \colon \Sigma \times \mathbb{R}^{M+1} \to \mathbb{R}_+$ Carathéodory functions,
$k^\Sigma_{\alpha\beta}(x, y) \geq c_R > 0$ f.a.a. $x \in \Sigma$, $\forall y \in \mathbb{R}^{M+1}$ with $y_0 \in [-R, R]$

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additional growth conditions for the source terms in reactions and boundary terms